PR-2. CHEMISTRY USING COMPUTER AS TEST TUBE

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Three different reactions related to chemistry (nucleophilic substitution reaction, redox reaction and reaction catalyzed by surface) would be discussed using density functional theoretical (DFT) methods. Investigation of products formation [1] of N-benzyl-2-chloro-3-nitroquinoline-4-amine and N, N-dibenzyl-3-nitroquinoline-2,4-diamine from the reaction of 2,4-dichloro-3-nitroquinoline and benzyl amine in the presence of neat solvent as well as in water, DMF, methanol and toluene using DFT with different functionals (B3LYP, M06-2X and APFD) and different Pople basis sets (6-31G(d), 6-311+G(2d, p)). We have carried out transition state calculations for the three possible products as N-benzyl-2-chloro-3-nitroquinoline-4-amine (para), N-benzyl-4-chloro-3-nitroquinoline-2-amine (ortho) and N, N-dibenzyl-3-nitroquinoline-2,4-diamine (ortho-para). In comparison to ortho and para products, para product is more favorable as the reaction rate is found to be more in case of para. Along with that the effect of solvent is also found approximately double in case of methanol and DMF for para products which might be attributed to polarity of the solvent and the stability of the transition state.

Understanding of Challenger's reductive/oxidative methylation pathway of arsenic metabolism [2] using DFT.

Molecular hydrogen, H2, is one of the fundamental constituents of the universe, acting as the molecular feedstock for much of the chemistry occurring within the interstellar medium [3]. Although gas phase models of the chemistry of interstellar clouds have been successful in explaining the abundances of some gas phase molecules, it has long been established that they cannot account for the large abundance of molecular hydrogen. The general consensus of the astronomical community is carbonaceous interstellar dust grains assume a catalytic role in the formation of H2 molecules within interstellar clouds [4]. Furthermore, the collinearly-dominated Eley-Rideal H2 formation pathway has been studied using quantum dynamics.

References

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